

Forms of Approximate Radiation Transport

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Photon radiation transport is described by the Boltzmann equation. Because this equation is difficult to solve, many different approximate forms have been implemented in computer codes. Several of the most common approximations are reviewed, and test problems illustrate the fundamental characteristics of each approximation.

Introduction

The Boltzmann transport equation describes how a variety of different types of particles travel through a material. It is generally considered the most accurate description of the statistical average density of particles in a system, as long as the particles do not interact with themselves. In radiation transport, the photon interactions with material can be described by a coupled set of equations (Pomraning, 1973; Zel'dovich and Raizer, 2002), namely

$$\frac{1}{c} \frac{\partial I}{\partial t} + \boldsymbol{\Omega} \cdot \nabla I = \sigma_a (B(T_m) - I) \quad (1)$$

$$\frac{\partial u_m}{\partial t} = - \int_{4\pi} \sigma_a (B(T_m) - I) d\boldsymbol{\Omega} + Q_m \quad (2)$$

where $I(\mathbf{x}, \boldsymbol{\Omega}, t)$ is the intensity, ν is the frequency of the particles, $\boldsymbol{\Omega}$ is the direction of the particle travel, t is time, σ_a is the absorption opacity, u_m is the material energy density, $T_m(u_m)$ is the material temperature and is a function of the material energy, Q_m is an external source of material heating, and $B(T_m)$ is Planck's function. The one group, or gray, approximation has been assumed for simplicity.

The intensity I contains much more detailed information than is frequently needed to solve a particular problem. In fact, the coupling with the material in Eq. 2 is only through the integral of I over all angles. We can define the radiation energy density as

$$E = \frac{1}{c} \int_{4\pi} I d\boldsymbol{\Omega}. \quad (3)$$

Equations 1 and 2 form a nonlinear system, even if the material properties are constant. They can be quite difficult to solve, and an approximation to Eq. 1 is nearly

always made before solving the system. This paper reviews several of the most popular approximations used in the radiation transport community.

The Approximations

Equations 1 and 2 form a nonlinear system. They can be quite difficult to solve, and an approximation to Eq. 1 is nearly always made before solving the system. This paper reviews four of the most popular approximations used in the radiation transport community.

The diffusion equation is very easy to solve but is inaccurate in optically thin regions and where the gradient of the energy density is large. Flux limited diffusion is an improvement to fix these deficiencies at the cost of making the equations nonlinear. Diffusion and P_1 are very closely related; variable Eddington factor approximations are a nonlinear improvement upon the P_1 approximation, much in the same way that flux limited diffusion improves upon regular diffusion.

The equations that arise in the discrete ordinates (S_N) approximation are also very easy to solve, especially in serial calculations. Recent work has gone into making S_N work on unstructured meshes in parallel. The most severe problem that S_N has is the inclusion of artifacts in the solution called ray effects.

The spherical harmonics approximation (P_N) has been around for a long time, but has not gotten much use in large codes. While S_N suffers from ray effects, P_N suffers from wave effects in time dependent problems

Monte Carlo is not an approximation of the transport equation. While the transport equation describes the statistical average of the particles in the system, Monte Carlo methods try to build up an average by simulating many individual particles. Because it is infeasible to simulate as many particles as there are in the physical system, the accuracy of the solution is usually limited by computer time and memory.

Only the Boltzmann equation, Eq. 1, is being approximated in all these methods; the material energy equation, Eq. 2, is unchanged.

Diffusion

For many problems, only the energy density E is important. In fact, it is this quantity that shows up in Eq. 2. Instead of solving for I directly and then integrating over angle to compute E indirectly, we can manipulate Eq. 1 to yield an equation for E instead of I .

The diffusion equation and the material equation are

$$\frac{1}{c} \frac{\partial E}{\partial t} - \nabla \cdot D \nabla E = \sigma_a (B(T_m) - E), \text{ and} \quad (4)$$

$$\frac{\partial u_m}{\partial t} = c \sigma_a (E - B(T_m)) + Q_m, \quad (5)$$

where D is the diffusion coefficient.

There has been a fundamental change in the form of the equations; the transport equation (Eq. 1) is hyperbolic, implying that particles (and energy) travels at finite speeds, but the diffusion equation is parabolic, allowing the particles to travel at infinite speed; a small change in one part of the problem immediately affects every other part of the problem.

Flux Limited Diffusion

A large source of problems with the diffusion approximation comes from the fact it allows $|\eta| > 1$, where

$$\eta \equiv \frac{\mathbf{F}}{cE}. \quad (6)$$

This is completely unphysical; it implies that more energy can be moving than exists at a point to begin with, or, in other words, the flux \mathbf{F} is not limited by the energy density. To correct this problem, various forms of the diffusion coefficient, D , have been proposed in order to limit the flux. Many different flux limiters have been proposed (Olson et al., 2000; Su, 2001).

Flux limited diffusion is nearly as cheap as regular diffusion to compute, and much, much cheaper than any of the higher order approximations. This accounts for its extraordinary popularity and usefulness for the foreseeable future.

Discrete Ordinates

The discrete ordinates approximation assumes that particles can only travel along a few particular directions, instead of the infinite number of directions allowed in Eq. 1. These directions are generally chosen to be symmetric for any ninety degree rotation of the coordinate system. Mathematically, this approximation assumes that the intensity is a sum of delta functions,

$$I(\mathbf{r}, \boldsymbol{\Omega}, \varepsilon, t) = \sum_{n=1}^M I_n(\mathbf{r}, \varepsilon, t) \delta(\boldsymbol{\Omega} - \boldsymbol{\Omega}_n). \quad (7)$$

If we insert this into Eq. 1, we find that we have N different equations, one for each direction (or ordinate) $\boldsymbol{\Omega}_n$,

$$\frac{1}{c} \frac{\partial I_n}{\partial t} + \boldsymbol{\Omega}_n \cdot \nabla I_n = \sigma_a (B(T_m) - I_n) \quad (8)$$

where w_m is an integration weight. Each direction n is coupled to all the others through the material equation. Eq. 8 can be differenced in an upwinded manner, leading to a very efficient solution algorithms.

The discrete ordinates approximation in more than one spatial dimension has a well-known defect called ray effects (Lewis and Miller, 1993; Miller and Reed, 1977). Due to the discrete nature of the angular approximation, particles do not reach regions where they otherwise would, sometimes producing large spatial oscillations in the energy density E .

The N in the abbreviation S_N comes from the quadrature order. In one dimension, the quadrature order is equal to the number of directions in Eq. 7. In two and three dimensions, the number of directions is proportional to N^2 .

Spherical Harmonics

The intensity, I , can be expanded with a set of orthonormal functions called the spherical harmonic functions,

$$I(\mathbf{r}, \boldsymbol{\Omega}, \varepsilon, t) = \frac{c}{\sqrt{4\pi}} \sum_{l=0}^{\infty} \sum_{m=-l}^l E_l^m(\mathbf{r}, \varepsilon, t) Y_l^m(\boldsymbol{\Omega}) \quad (9)$$

$$E_l^m(\mathbf{r}, \varepsilon, t) = \frac{\sqrt{4\pi}}{c} \int_{4\pi} \bar{Y}_l^m(\boldsymbol{\Omega}) I(\mathbf{r}, \boldsymbol{\Omega}, \varepsilon, t) d\boldsymbol{\Omega}, \quad (10)$$

where E_l^m is the moment of I with respect to the spherical harmonic function Y_l^m . The lowest order spherical harmonic $Y_0^0 = 1/\sqrt{4\pi}$, so the multiply and divide by $\sqrt{4\pi}$ in Eq. 9 and Eq. 10 is so that $E_0^0 = E$ is the energy density. The P_N approximation arises when it is then assumed that if $l \geq N$, then moments $E_l^m = 0$.

If we multiply Eq. 1 by each \bar{Y}_l^m , the complex conjugate of Y_l^m , and integrate over angle, we get a series of equations for the moments of the intensity I . Each moment E_l^m is only coupled to the moments $E_{l'}^{m'}$, where $l' = l \pm 1$ and $m' = m + \{-1, 0, 1\}$, for a total of six other moments. This system of equations can be written in vector form as

$$\frac{1}{c} \frac{\partial \mathbf{E}}{\partial t} + \mathbf{A}_x \frac{\partial \mathbf{E}}{\partial x} + \mathbf{A}_y \frac{\partial \mathbf{E}}{\partial y} + \mathbf{A}_z \frac{\partial \mathbf{E}}{\partial z} = -\sigma_t \mathbf{E} + \mathbf{S}, \quad (11)$$

where \mathbf{A}_i are the Jacobians with respect to the i^{th} direction describing the details of how the moments are coupled, \mathbf{E} is a vector of the moments E_l^m , and \mathbf{S} is the source vector and contains the scattering and material emission terms. The Jacobians \mathbf{A}_i are constant in space and share a remarkable property—the eigenvalues of each matrix are identical. Particles travel in waves through the system at a finite number of speeds determined by these eigenvalues. The more moments, the more eigenvalues, the more different speeds,

and the more accurate the solution can be. As for S_N , the number of unknowns is $N + 1$ for one dimension, and is proportional to N^2 in two and three dimensions.

The spherical harmonics approximation has a not-so-well-known defect called wave effects in the time dependent case. In a vacuum, the system of equations is a wave equation, and it is possible to get negative energy densities $E = E_0^0$. This is clearly unphysical. Not only is this important for vacuum regions, but on short time scales, interactions with the material become unimportant, and the equations again look like they are in a vacuum. Even in time dependent problems without voids, it is possible to get a negative solution for the energy density E . The energy density in steady state problems is always nonnegative.

Monte Carlo

The Boltzmann transport equation (Eq. 1) and approximations based on it solve for the statistical average of energy densities. It treats the radiation as a continuous field; particles do not really exist.

Monte Carlo, on the other hand, embraces the particle as its fundamental feature. Individual photons are simulated from birth to death, modifying the material energy as they travel. When a simulated photon is emitted from the material, it slightly decreases the material energy. This photon travels through the model, occasionally interacting with the material through scattering or absorption events. When the photon is absorbed, the material energy is incremented a little bit.

All of the photon's interactions, including its birth, have certain probabilities of occurring that we can estimate. A pseudo random number generator is used in conjunction with these probabilities to calculate when, where, and what kind of event occurred. Once many particles have been simulated, a reasonable average for the energy density is estimated.

The biggest disadvantage of Monte Carlo is that it is both processor time and memory intensive; otherwise, it generally yields very accurate results, once enough particles have been simulated. The estimated error in the Monte Carlo calculation is

$$\text{Error} = \frac{\alpha}{\sqrt{N}}, \quad (12)$$

where α is some proportionality constant and N is the number of particles simulated. This equation implies that in order to achieve a factor of 10 decrease in the estimated error, 100 times more particles need to be simulated. There are many variance reduction techniques that can be used to dramatically reduce the proportionality constant α , but the general scaling of error with the number particles simulated shown in Eq. 12 still applies. While deterministic approximations (diffusion, S_N , P_N) have a uniform error throughout the system, the Monte Carlo simulation has the largest error where there are the fewest particles. The deterministic approximations get equally good (or bad) results everywhere.

In very rare instances, the simulation can produce a completely wrong result, especially if something important happens where there are not very many photons. Consider the case of a supercritical nuclear reactor behind a very thick neutron shield. Since pure uranium is not an emitter of neutrons, there is nothing to initiate run-away chain reaction in the reactor, except for the source of neutrons on the other side of the shield. A Monte Carlo simulation might not ever transport a neutron to the reactor, giving you a false sense of security. In the real world, there would be so many neutrons, the probability that at least one will reach the reactor is very great.

A Few Test Problems

The problems in this section are designed to give some insight as to how the various approximation perform relative to each other. Some of the problems are a test of neutral particle transport; they are not coupled to the material energy at all. All of the calculations are single-group in energy.

A Line Source in Two Dimensions

The most basic of all time dependent problems is a Green's function problem. In two dimensions this is a pulse of particles is emitted from a line source. In a linear system such as ours without the material equation, solutions to all other time dependent problems are just superpositions of solutions of different Green's function problems. Only a vacuum is considered here; there is no coupling with the material. This test problem is designed to show the fundamental differences in each of the approximations. The defects in each of the approximations that are exposed by this problem will also be seen in all of the other test problems considered in later sections.

The energy density can be solved for analytically for most approximations. Solving the transport equation, Eq. 1, for the intensity I , then integrating over angle to get the energy density E yields

$$E^{\text{transport}} = \frac{E^0}{2\pi} \frac{h(ct - r)}{ct\sqrt{c^2t^2 - r^2}}, \quad (13)$$

where E^0 is the strength of the initial radiation pulse along the line and $h(x)$ is the unit step function. The general P_N solution is

$$E^{P_N} = \frac{E^0}{\pi} \sum_{\lambda_i \geq 0} r_i l_i \left[\frac{\delta(r - \lambda_i t)}{\sqrt{\lambda_i^2 t^2 - r^2}} - \frac{\lambda_i t h(\lambda_i t - r)}{(\lambda_i^2 t^2 - r^2)^{3/2}} \right], \quad (14)$$

Note that there are regions where the solution for E^{P_N} is negative. This is an essential defect of the P_N equations, not a problem with the numerical implementation. The

general S_N solution is

$$E^{S_N} = E^0 \sum_i w_i \delta(\|\mathbf{x} - ct\boldsymbol{\Omega}_i\|), \quad (15)$$

where the sum over i denotes a sum over all angles. In contrast to the transport and P_N solutions, the S_N solution is a function of both x and y instead of a function of r only. This rotational dependence of the discrete ordinates equations is a factor in the problem called ray effects. In the diffusion case, there is no solution. Eq. 4 is not well defined in a vacuum. The nonlinear (and therefore much harder to solve analytically) flux limited diffusion is defined in a vacuum, and the numeric solution is shown in Figure 1(e).

Figure 1 shows various numerical solutions for the line source problem. All simulations are on a grid two centimeters square with a mesh spacing of about $dx = 0.01$ cm. The Monte Carlo simulation in Figure 1(b) is very similar to the transport solution in Figure 1(a), with the exception statistical noise in the solution. This simulation used one hundred thousand particles. It is fairly easy to reduce this noise by simply increasing the number of particles in the simulation. Figure 1(c) and Figure 1(d) show the P_1 and P_5 solutions, respectively. The P_1 approximation has one wave speed at which particles can travel, whereas P_5 has three wave speeds. This can be seen in the rings moving away from the center. Just behind each ring, there is a negative region in the energy density. Figure 1(e) is not a mistake. The distribution spread out so fast that the distribution is essentially flat and has a very small and nearly uniform value everywhere. A discrete ordinates S_6 calculation is shown in Figure 1(f). Note that the particles are all moving in delta functions away from the center.

The full transport equation is hyperbolic in nature, which means that particles and information can only travel at finite speeds. All of the approximations except diffusion respect this; all of the approximation in Figure 1 have semi-reasonable¹ answers except the diffusion. The key difference between spherical harmonics (P_N) and discrete ordinates (S_N) is that S_N moves particles around along particular beams, giving rise to ray-effects; while P_N moves particles only with particular speeds, giving rise to wave-effects. The Monte Carlo simulation looks the best, but if the problem would have been sensitive to instabilities, the noise in the simulation could be problematic.

A Lattice Problem

This problem is a checkerboard of highly scattering and highly absorbing regions loosely based on a small part of a nuclear reactor core. This is only a test of the transport approximations; there is no material energy equation. When an absorption occurs, the particles are simply removed from the system and do not heat it up.

¹A “semi-reasonable” answer is one that converges to the correct solution as the order of the method is increased; the results shown in Figures 1(c)-1(f) are by no means truly reasonable.

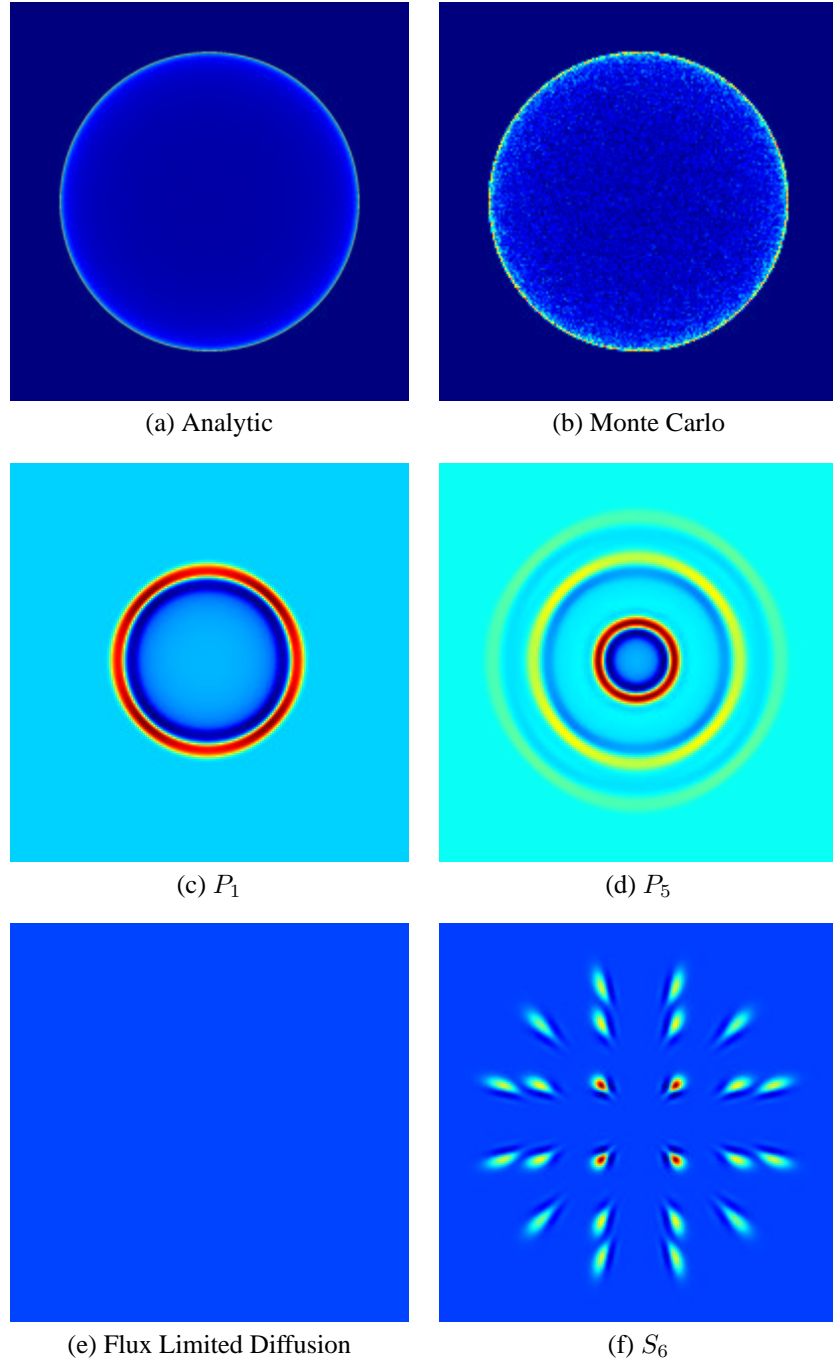


Figure 1. Solutions to the pulsed line source problem. The color scale is linear, and the color at each of the corners equals zero for all approximations except diffusion which uses the same scale as S_6 . Colors more blue than the corners are negative.

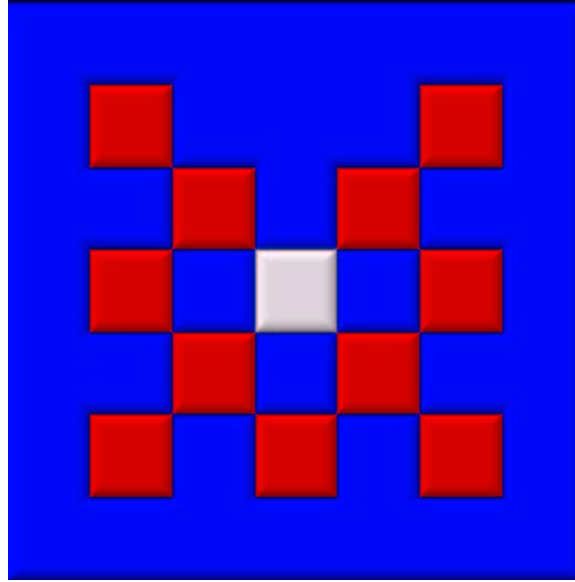


Figure 2. The lattice system. The blue and white regions are pure scattering regions where $\sigma_s = 1 \text{ cm}^{-1}$. Additionally, the white region contains a source of particles. The red regions are pure absorbers with $\sigma_a = 10 \text{ cm}^{-1}$. The particles are simply removed from the system by the absorbers; there is no material equation.

The system for this problem, shown in Figure 2, is seven centimeters wide. The bulk of the lattice is composed of a scattering material with $\sigma_t = \sigma_s = 1 \text{ cm}^{-1}$. There are eleven absorbing regions where $\sigma_t = \sigma_a = 10 \text{ cm}^{-1}$. At time zero, a source of strength one is turned on in the central region of the system. All particles travel at a speed $c = 1 \text{ cm/s}$, and the problem is surrounded on all sides by vacuum boundaries.

Figure 3 shows the energy density 3.2 seconds after the source is turned on . using diffusion, flux limited diffusion, P_1 , P_7 , S_6 , and implicit Monte Carlo approximations. The diffusion and the discrete ordinates calculations were done with ALEGRA (Brunner and Mehlhorn, 2004). The implicit Monte Carlo calculation was done using the KULL IMC package (Gentile et al., 1998; Gentile et al., 2005; Brunner et al., 2005) and used thirty six million particles in half the problem domain, with a reflective boundary on the center line. The P_N calculations were done with a research code of my own (Brunner, 2000; Brunner and Holloway, 2005).

The particles should have had just enough time to reach the boundaries but not enough to reach the corners. The diffusion calculation shown in Figure 3(a) is much too diffuse; the particles have reached all parts of the system. Also, the central region does not have enough particles. The flux limited diffusion result in Figure 3(b) is a vast improvement

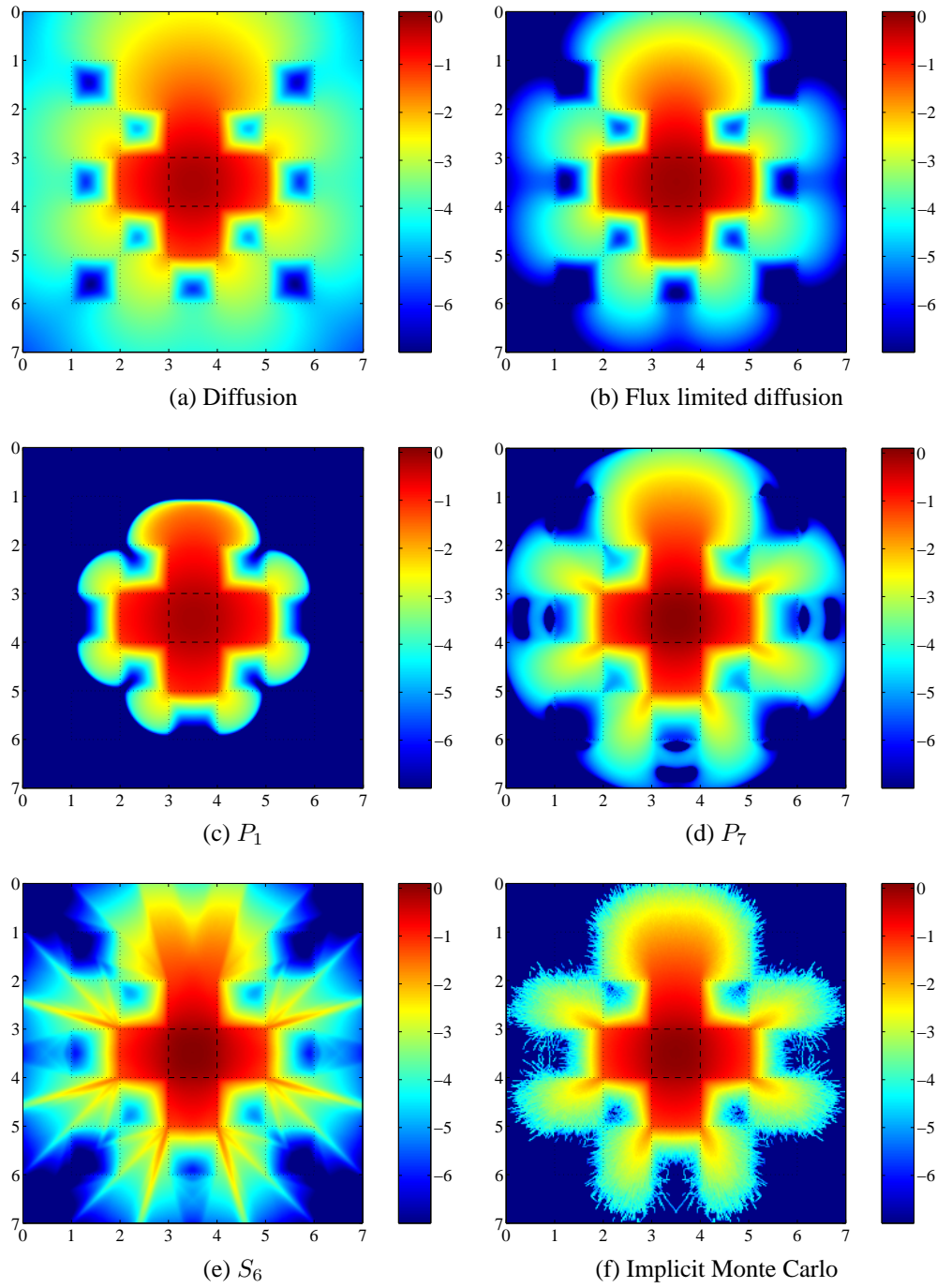


Figure 3. The calculated energy density in the lattice problem 3.2 seconds after the source was turned on. The color-map is proportional to $\log_{10} E$ and limited to seven orders of magnitude.

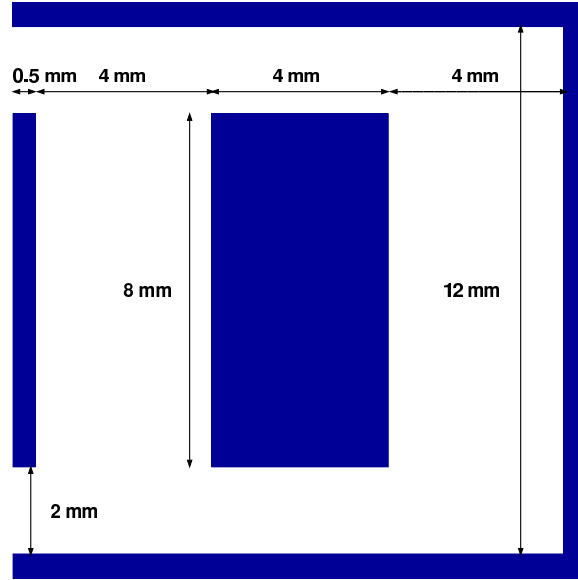


Figure 4. The hohlraum. The blue regions are pure absorbers regions where $\sigma_a = 100 \text{ cm}^{-1}$ and $\rho C_v = 5.0 \times 10^5 \text{ J/m}^3 \text{ K}$. The white region is a vacuum.

upon the diffusion calculation and captures the wave front well, but there are no beams of particles leaking between the absorbers as seen in the Monte Carlo and P_7 calculations. The energy density computed using P_1 , seen in Figure 3(c), has an artificial wave front of particles traveling at speed $v = 1/\sqrt{3} \text{ cm/s}$. This is due to the fact that in P_1 , the particle waves travel only at this speed. In the P_7 calculation, the particle waves can travel at more speeds, nearly eliminating these nonphysical wave fronts. Some wave-effects can also be seen in the P_7 calculation. Well defined beams of particles leaking between the corners of the absorbing regions in both Figure 3(d) and Figure 3(f), the P_7 and Monte Carlo simulations. Generally P_7 and Monte Carlo agree very well, especially for energy densities above 10^{-4} . The S_6 calculation shown in Figure 3(e) has about the same number of degrees of freedom as the P_7 calculation, but the ray-effects are very dominant.

A Hohlraum

This hohlraum problem is loosely based on a typical hohlraum for the Z-machine at Sandia. The radiation field is coupled to the the material energy through Eq. 2. Unlike a real hohlraum, this problem is described in Cartesian coordinates. The system, shown in Figure 4, is thirteen millimeters square with a thin wall of material around the outside edge. There are two two millimeter openings on either left side of the hohlraum, and there is a rectangular block of material in the center of the system. The material is a pure

absorber with $\sigma_a = 100 \text{ cm}^{-1}$ and $\rho C_v = 5.0 \times 10^5 \text{ J/m}^3 \text{ K}$. The rest of the problem is a vacuum. Some codes used for this problem could not model a pure void, so the heat capacity was set extremely large, $\rho C_v = 1.0 \times 10^{99} \text{ J/m}^3 \text{ K}$. The opacities were all set to zero in the void. The initial material and radiation temperatures were set to $T_0 = 300 \text{ K}$. A source boundary condition is applied along the entire left hand side. The source has a temperature of $T_{\text{source}} = 3.5 \times 10^6 \text{ K}$.

Figure 5 shows the radiation temperature at $t_1 = 3.93606 \times 10^{-11} \text{ s}$. Throughout the discussion below, it is assumed that the Implicit Monte Carlo simulation is the most accurate answer.

At the time depicted in Figure 5, photons have had nearly enough time to back wall of the hohlraum. Most of the photons are still streaming from the openings; the walls of the hohlraum have not started to heat up yet. Flux limited diffusion, Figure 5(b) has incorrectly allowed photons to fill the entire system. The P_9 (Figure 5(c)) simulation has wave-like solutions, which allow the photons to bend around the front wall. Notice the black regions in the P_9 solution in Figure 5(c); these represent negative solutions. While too many photons are transported in the wave front around the back side of the wall, P_9 “tries” to compensate by having waves of negative energy follow the positive waves that should not be there. The S_8 calculation suffers badly from ray-effects. While these ray-effects persist even at long times, the wave effects seen in P_9 solution, Figure 5(c), quickly travel through the system.

Conclusions

Simulating radiation transport is difficult; the equation we would really like to use, the Boltzmann transport equation, is seven dimensional. This leads to a myriad of different approximations to the transport equation.

Diffusion is by far the simplest approximation and works well when there is material for the photons to diffuse through. The many varieties of flux limited diffusion all attempt to improve upon plane diffusion while remaining fairly easy to solve. The errors with diffusion theory all stem from the fact that the fundamental mathematical characteristic of the transport has been changed from hyperbolic to parabolic. This change means that photons are no longer constrained to travel at the speed of light. Some extremely fast and robust numerical methods have been developed to numerically solve the diffusion theory equations.

The spherical harmonics approximation takes moments of the Boltzmann equation to arrive at a set of conservation laws for each of the moments. In a vacuum, this approximation leads to the wave equations, and this causes the simulations to suffer from wave-effects. Theoretically these effects become negligible when enough moments are used, but in a vacuum, an infinite number of moments are needed to eliminate the

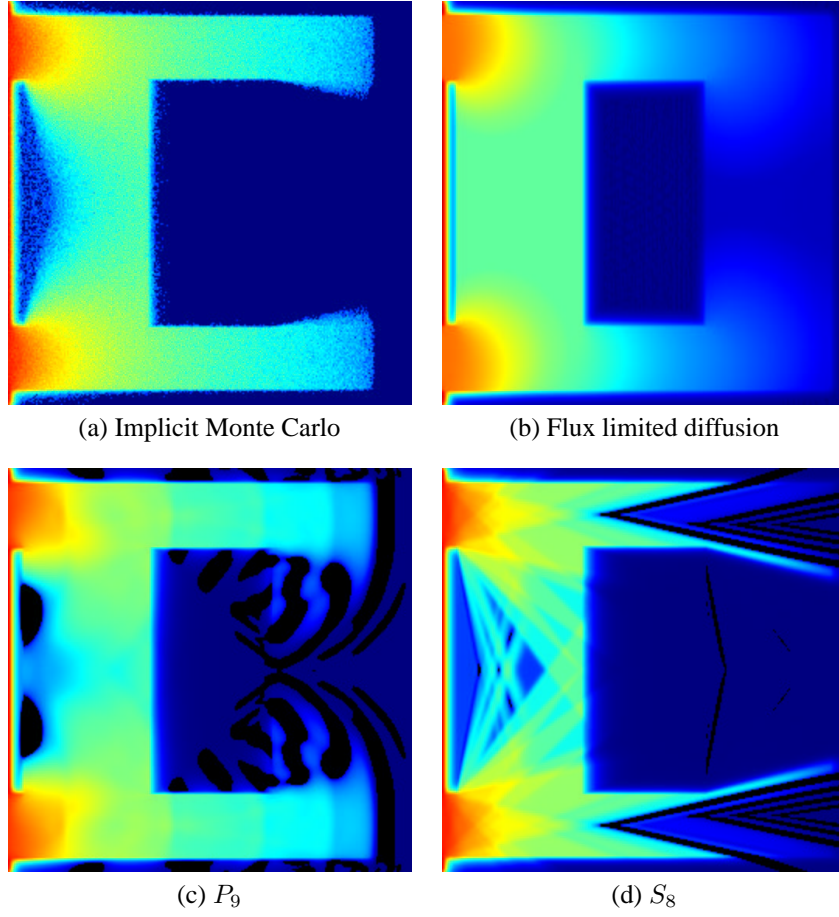


Figure 5. The radiation temperature in the hohlraum problem at $t = 3.93606 \times 10^{-11} \text{ s}$ after the source was turned on. The color-map is proportional to $T_r = (E/a)^{1/4}$. Black regions indicate negative energy densities.

wave-effects.

The discrete ordinates approximation moves photons only along a particular set of directions. Many people have studied this approximation, making its problems well understood. Many very efficient algorithms have been developed to solve the discrete ordinates equations. Unfortunately, ray-effects, the most well-known defect of discrete ordinates, can be seen in many simulations.

Implicit Monte Carlo can treat photons exactly, but a given simulation cannot come close to simulating as many particles as there are in all physical systems. This leads to statistical noise, which is this method's largest weakness. In order to reduce the amount of noise in a given simulation by a factor of ten, one hundred times more particles must be simulated. In time-dependent problems, not only does this increase run-time by a factor of one hundred, but memory usage also increases by the same factor. The resulting material energy calculated in an Monte Carlo simulation, however, is much less noisy than the radiation field, and it is usually the material energy that is more important for simulations.

For the test problems in this paper, the Monte Carlo generally gave the best results. Flux limited diffusion gave the best results normalized by run time. Spherical harmonics and discrete ordinates both have some significant problems in optically thin materials, but spherical harmonics appears to perform slightly better in highly heterogeneous material such as the lattice problem.

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